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THE INTERACTION OF DISLOCATIONS AND RADIATION-INDUCED OBSTACLES AT HIGH-STRAIN RATE

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Abstract. Improved understanding of the plastic deformation of metals during high strain rate shock loading is key to predicting their resulting material properties. This paper presents the results of molecular dynamics simulations that identify the deformation modes of aluminum over a range of applied shear stresses and examines the interaction between dislocations and irradiation induced obstacles. These simulations show that while super-sonic dislocation motion can occur during impact loading, the finite dimensions of the materials render this motion transient. Larger applied loads do not stabilize supersonic dislocations, but instead lead an alternate deformation mode, namely twinning. Finally, the atomistic mechanisms that underlie the observed changes in the mechanical properties of metals as a function of irradiation are examined. Specifically, simulations of the interactions between moving edge dislocations and nanometer-sized helium bubbles provide insight into increases of the critical shear stresses but also reveal the effect of internal gas pressure on the deformation mode. The information gained in these studies provides fundamental insight into materials behavior, as well as important inputs for multi-scale models of materials deformation.

INTRODUCTION

Computer simulations are currently capable of providing new insights into fundamental mechanisms of materials deformation at the atomic and nano-scale, as well as predictions of material properties. For example, the study of plastic deformation of metals during shock loading yields insights into the fundamental behavior of dislocation and atomic deformation mechanisms controlling plastic deformation. Traditionally, it has been thought that dislocations could not move faster than the speed of sound, yet recent simulations have shown the existence of supersonic dislocations under high-applied strains[1]. One of the questions to be addressed in this paper is the subsequent stability of these dislocations.

The stress regime required to nucleate supersonic dislocations also lends itself to the activation of deformation modes otherwise inaccessible under quasi-static deformation. For example, high stacking fault energy materials, such as aluminum, have high critical stress for deformation twinning. These high stresses render experimental examination of the deformation details difficult at best, therefore, this paper presents results which identify alternate modes of deformation and their atomistic origins.

Materials, especially those exposed to radiation or utilized in aggressive corrosive or thermally-cycled environments, are not defect free. While many of the basic physical mechanisms governing irradiation induced hardening or environmentally-assisted degradation are understood, it is still unclear what mechanisms are dominant under specific conditions. Likewise many multi-scale models require accurate estimates of key material parameters. For example, the interaction between dislocations and nanometer voids and/or helium bubbles that form during irradiation, are known responsible for increased strength and decreased ductility; the manner in which factors such as the number density, size and internal pressure, these defects determine the final material properties remain to be determined. It is for these reasons that we will examine the interactions between edge dislocations in aluminum and He bubbles over a range of internal gas pressure.

PROCEDURE

Molecular dynamics (MD) simulations are an ideal tool to investigate deformation phenomena at high-strain rates, since they directly account for core and non-linear effects ignored by elastic theory. The motion of edge dislocations and their interactions with obstacles in aluminum has been studied using the molecular dynamics code MDCASK[2]. The simulation system used in our simulations has basis vectors along the $X=[\bar{1}11]$ Y=[110] and $Z=[1\bar{1}2]$ directions. Periodic boundary conditions are used in the Y and Z directions while the $X=[\bar{1}11]$ faces are free surfaces. Each system contains approximately one million atoms. The Ercolessi and Adams force-matching embedded atom method potential[3] is used to model the aluminum/aluminum interactions while pair potentials are used for the aluminum/helium interactions[4] and helium/helium interactions.

An edge dislocation is introduced into the cell by removing two (220) half planes. For studying the dislocation interactions with radiation-induced obstacles, helium bubbles are introduced into the center of the cell by removing a 2.6 nm diameter sphere of atoms and introducing the desired number of helium atoms. Helium/lattice site ratios of 0.0 (i.e. a void), 0.5, 1.0 and 2.0 are considered. Dislocation motion is then studied as a function of applied shear stress by applying a constant surface traction in the [110] direction to the atoms in the two $(\bar{1}11)$ surfaces. The range of applied stresses from 25 MPa to 1000 MPa, corresponding to 0.15% to 3.0% of the shear modulus is covered in this work.

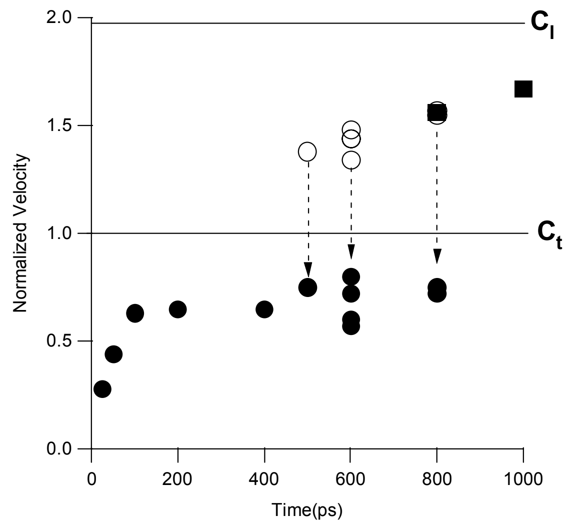

FIGURE 1 The velocity and deformation mode as a function of applied shear stress. Glide deformation is denoted by circles, open circle indicate transient velocities and closed circles indicate stable steady-state velocities, and squares indicate twinning.

RESULTS/DISCUSSION

Both the rate of plastic deformation and the mode of deformation are important in determining the mechanical properties of a metal. This is particularly true at high strain rates were deformation modes not accessible to a material under normal quasi-static deformation may be activated. Figure 1 summarizes the steady-state velocities of edge dislocations over a range of applied shear stresses. For applied shear stresses of up to 500 MPa, classic velocity/stress relationships are seen. These include the linear region (25 MPa-100 MPa) where frictional forces limit the velocity of the dislocation as well as the plateau region (100 MPa-400 MPa) where the velocity is limited by the transverse sonic wall. The saturation velocity of 2350 m/s corresponds to approximately 68% of the transverse sound speed, C_t, yielding a strain rate of ~$1x10^8$ s^{-1}. For the parameters of this interatomic potential for aluminum, the transonic sound speed is $C_t \approx$ 3475 m/s.

Higher applied stresses produce trans-sonic dislocation motion. Figure 1 plots the velocity of dislocations as a function of applied stress and shows not only that transonic dislocations are transient but that twin deformation is also activated at high stress. To investigate the origin of the transonic instability we begin by examining the case in which the trans-sonic dislocation slows to a steady subsonic velocity while maintaining dislocation glide.

Examination of the position of the dislocation and the stacking fault width as a function of time for different size cells (X=50 and X=80 lattice units), is plotted in Figure 2 and shows that the existence of the free surfaces are responsible for the slowing of the dislocation. Specifically, it takes 0.5 X/C_t ps, traveling at the speed of sound, for the applied shear stress to be transmitted to the dislocation that is located in the center of the cell and initiate transonic motion. It takes an additional 1.0 X/C_t ps for the wave composed of the applied stress and the shock wave excited by the transonic dislocation to reach the free surface, excite surface waves and arrive back at the dislocation. Thus, an interaction between the transonic dislocation and the surface waves occurs 1.5 X/C_t ps after application of the applied stress and causes the slowing of the dislocation to a steady-state subsonic saturation velocity. As seen in figure 2, the breaking effect of the surface wave is manifested through an increase in the width of the stacking fault at the time 1.5X/Ct. Shortly thereafter, the partial dislocations recover their equilibrium spacing at a stable subsonic velocity. These simulations provide direct evidence that while dislocations can be accelerated to transonic speeds as a result of high-strain rate impulse loading, the excitation of Rayleigh waves from internal surfaces and interfaces will rapidly result in steady-state dislocation motion at a subsonic saturation velocity[5].

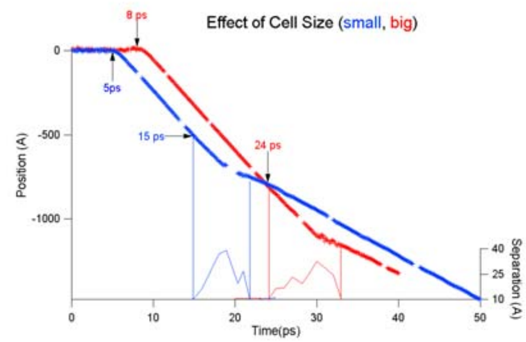

FIGURE 2. The average position of the dislocation and the separation of the partial dislocations (stacking fault width) as a function of time following an applied shear stress of 600 MPa. The applied shear wave reaches the dislocation after 5ps and 8 ps for the small and large cells respectively.

It is also important to note that at these high strain rates another deformation mode becomes accessible, namely deformation twinning. These simulations reveal that nano-twin formation results from the homogenous nucleation of dislocation dipoles along the stacking fault. While this is not an anticipated deformation mode for aluminum due to a high stacking fault energy, 110-130 mJ/m^2, similar results have been published for nano-crystalline aluminum[6].

Atomistic simulations of the interaction between moving edge dislocations and 2.6nm helium bubbles as a function of internal gas pressure provide information key material behavior parameters. Estimates of critical angles and stresses are central to models such as Orowan's theory of dispersed obstacle hardening[7]. Helium bubbles having He/lattice ratios of 0-1 shear as a result of interaction with the dislocation. The bubbles are sheared by one Burger's vector with the passage of each dislocation. A critical stress of less than 25 MPa has been determined for the void and 35 MPa for the He/lattice=0.5 bubble. This value is in reasonable agreement with critical stresses obtained from TEM observations of irradiated copper[8].

At higher pressures corresponding to He/lattice= 2.0 a different interaction is seen. In this case the internal pressure of the bubble creates a significant disruption of the aluminum lattice. As the dislocation interacts with the bubble it not only shears the bubble, but also adsorbs vacancies, resulting in dislocation climb with the formation of a pair of less mobile super jogs. These super jogs then act to reduce the glide mobility of the edge dislocation. These results indicate that in irradiated metals the internal pressure of the bubbles not only determines the critical stress but also the mechanism by which dislocations interact with the obstacles and the rate of plastic deformation.

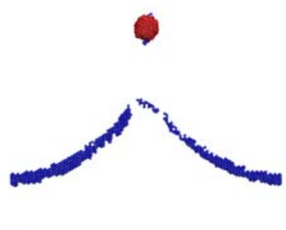

FIGURE 3. The jogged dislocation which results from interaction with a bubble having He/lattice=2.0. The blue spheres define the dislocation and the red spheres represent helium atoms.

SUMMARY AND FUTURE WORK

The results presented in this paper address various aspects of materials deformation at high strain rates. Specifically, the motion of super-sonic dislocations has been shown to be transient resulting from the finite dimensions of the material. While twinning in aluminum is difficult to observe experimentally, these simulations reveal the onset of twin deformation by homogenous partial dislocation dipole nucleation at shear stresses of 800 MPa. Finally, both the critical stress and the interaction between a dislocation and He bubbles in irradiated metals is shown to depend of the internal gas pressure. Future work will involve additional simulations to examine the effect of dislocation morphology (i.e. screw dislocations) as well as the geometry of the dislocation/obstacle interactions.

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